

Diethyl propanedioate  
105-53-3 | DTXSID7021863

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

## Model Results

**Predicted value:** 2.90e-01 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 7.65e-01

**Confidence level:** 8.71e-01

## Nearest Neighbors from the Training Set

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Acetic acid, chloro-, 1-methylethyl ester

**Measured:** 2.69e-01

**Predicted:** 6.23

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4-Bromophenol

**Measured:** 4.10e-01

**Predicted:** 2.33e-02

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Benzene, (iodomethyl)-

**Measured:** 3.00e-01

**Predicted:** 1.97e-01

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N-Methoxymethylamine

**Measured:** 1.80e-01

**Predicted:** 122

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1,2-Phenylenediamine

**Measured:** 4.14e-01

**Predicted:** 8.53e-04